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## A nonholonomic Newmark method

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### ABSTRACT

Using the nonholonomic exponential map, we obtain a new version of Newmark-type methods for nonholonomic systems (see also Jay and Negrut(2009) for a different extension). We give numerical examples including a test problem where the structure of reversible integrability responsible for good energy behaviour as described in Modin and Verdier (2020) is lost. We observe that the composition of two Newmark methods is able to produce good energy behaviour on this test problem.

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## 1. Introduction

In numerical integration, one of the most widely used methods in nonlinear structure dynamics is without any doubt the Newmark family of numerical methods [1], which also admits extensions to constrained systems (see [2]).

Briefly, a nonholonomic system is a mechanical system with external constraints on the velocities whose equations are obtained using the Lagrange-d'Alembert principle (see [3]). These systems are present in a great variety of engineering and robotic environments as for instance in applications to wheeled vehicles and satellite dynamics. In this paper, we will consider only the case of linear velocity constraints since this is the case in most examples, but the extension of our nonholonomic Newmark method to the case of nonlinear constraints, explicitly time-dependent systems and nonholonomic systems with external forces is completely straightforward.

The case of linear velocity constraints is specified by a (in general, nonintegrable) regular distribution  $\mathcal{D}$  on the configuration space  $Q$ , or equivalently, by a vector subbundle  $\tau_{\mathcal{D}} : \mathcal{D} \rightarrow Q$  of the tangent bundle  $TQ$  with canonical inclusion  $i_{\mathcal{D}} : \mathcal{D} \hookrightarrow TQ$ . Therefore, the admissible curves  $\gamma : I \subseteq \mathbb{R} \rightarrow Q$  must verify the following constraint equation

$$\gamma'(t) = \frac{d\gamma}{dt}(t) \in \mathcal{D}_{\gamma(t)} \text{ for all } t \in I.$$

The case of holonomic constraints occurs when  $\mathcal{D}$  is integrable or, equivalently, involutive. Observe that in this case, all the curves through a point  $q \in Q$  satisfying the constraints must lie on the maximal integral submanifold of  $\mathcal{D}$  through  $q$ .

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In this paper, we construct nonholonomic Newmark methods in the case where  $Q$  is  $\mathbb{R}^n$  and discuss the possibility of composing Newmark methods to obtain higher-order methods. At the end, we test them in some nonholonomic problems. According to [4], the reason why several numerical methods produce good energy behaviour is due to the fact that they preserve reversible integrability and most nonholonomic examples are precisely reversible integrable. The perturbed pendulum-driven CVT system is an example of an unbiased nonholonomic system since it is no longer reversible. The main result of the paper is that in one of our methods, the composition of two Newmark methods, we observed nearly preservation of energy with a similar behaviour to the nonholonomic leap-frog method [5,6]. Our result may help finding numerical methods for nonholonomic systems exhibiting better qualitative behaviour than those existing in the literature for unbiased examples as well as it may give some contribution to the understanding of the reason why there are methods that do preserve the energy in these examples. This, in fact, is one of the open problems in the area of geometric integration of nonholonomic systems.

The paper is structured as follows. In Section 2, we give a review of the Newmark method to integrate second-order differential equations and rewrite them in terms of a discretization of the exponential map. In Section 3, we review the definition of nonholonomic mechanics and of the nonholonomic exponential map which motivates the introduction of nonholonomic Newmark methods. In Proposition 3.6, we prove that Newmark methods with  $\beta = \beta' = 0$  are equivalent to a DLA method and in Proposition 3.7, we obtain a numerical method from the composition of lower order Newmark methods. In Section 4, we give three examples of nonholonomic systems including the perturbed pendulum-driven CVT system and in Section 5 we present our numerical results. Finally, in Section 6, we discuss the possibility of generalizing nonholonomic Newmark methods to general manifolds and, in particular, to a Lie group (see [7]).

## 2. Newmark method for explicit second-order differential equations

Given a second order differential equation  $\frac{d^2q}{dt^2} = \Gamma(t, q, \dot{q})$  the classical Newmark method is given by

$$\begin{aligned} \frac{q_{k+1} - q_k}{h} &= \dot{q}_k + h \left( \frac{1}{2} - \beta \right) \Gamma(t_k, q_k, \dot{q}_k) + h\beta \Gamma(t_{k+1}, q_{k+1}, \dot{q}_{k+1}) \\ \frac{\dot{q}_{k+1} - \dot{q}_k}{h} &= (1 - \gamma) \Gamma(t_k, q_k, \dot{q}_k) + \gamma \Gamma(t_{k+1}, q_{k+1}, \dot{q}_{k+1}) \end{aligned} \tag{1}$$

where  $\gamma$  and  $\beta$  are real numbers with  $0 \leq \gamma \leq 1$  and  $0 \leq \beta \leq 1/2$ . The Newmark method is second order accurate if and only if  $\gamma = 1/2$ , otherwise it is only consistent. Moreover, this family of second order methods includes the trapezoidal rule ( $\beta = 1/4$ ) and the Störmer's method ( $\beta = 0$ ). In the latter case, the Newmark method is simplified as follows:

$$\begin{aligned} \frac{q_{k+1} - q_k}{h} &= \dot{q}_k + \frac{h}{2} \Gamma(t_k, q_k, \dot{q}_k) \\ \frac{\dot{q}_{k+1} - \dot{q}_k}{h} &= \frac{1}{2} \Gamma(t_k, q_k, \dot{q}_k) + \frac{1}{2} \Gamma(t_{k+1}, q_{k+1}, \dot{q}_{k+1}) \end{aligned}$$

### 2.1. Newmark method for Lagrangian systems

The Newmark method [1] is a classical time-stepping method that is very common in structural mechanical simulations. For simplicity, we consider a typical mechanical Lagrangian  $L : T\mathbb{R}^n \rightarrow \mathbb{R}$ :

$$L(q, \dot{q}) = \frac{1}{2} \dot{q} M \dot{q}^T - V(q), \tag{2}$$

where  $(q, \dot{q}) \in T\mathbb{R}^n \equiv \mathbb{R}^{2n}$ ,  $M$  is a symmetric positive definite constant  $n \times n$ -matrix and  $V$  is a potential function. The corresponding Euler-Lagrange equations are

$$\ddot{q} = -M^{-1} \nabla V(q), \tag{3}$$

where  $\nabla$  denotes the gradient of the potential function.

The Newmark methods are widely used in simulations of such mechanical systems. In fact, they can be applied in an even more general context including external forces (cf. [8]). In this case, fixing parameters  $\gamma$  and  $\beta$ , Eqs. (1) determine an integrator implicitly which gives  $(q_{k+1}, \dot{q}_{k+1})$  in terms of  $(q_k, \dot{q}_k)$  by

$$\begin{aligned} q_{k+1} &= q_k + h\dot{q}_k + \frac{h^2}{2} ((1 - 2\beta)a_k + 2\beta a_{k+1}) \\ \dot{q}_{k+1} &= \dot{q}_k + h((1 - \gamma)a_k + \gamma a_{k+1}), \end{aligned} \tag{4}$$

where  $a_k = -M^{-1} \nabla V(q_k)$  and  $a_{k+1} = -M^{-1} \nabla V(q_{k+1})$ .

In contrast with other geometric integrators for Lagrangian systems (see [9]), the Newmark scheme is not especially designed to be symplectic and momentum preserving, but in [8] the authors show that the conservation of the symplectic form and the momentum occurs in a non-obvious way. In other words, the Newmark methods preserve a non-canonical perturbed symplectic form and a non-standard momentum.

### 2.2. The Newmark method and the exponential map

Given a second order differential equation  $\frac{d^2q}{dt^2} = \Gamma(t, q, \dot{q})$  on  $Q$ , a point  $q \in Q$  and a sufficiently small positive number  $h > 0$ , we can construct the exponential map of  $\Gamma$  in  $q$  at time  $h$ , i.e., a map  $\exp_{q,h}^d : U \subseteq T_qQ \rightarrow Q$ . This map is defined taking for any vector  $v \in T_qQ$  the unique trajectory of the second order differential equation with this initial condition, that is the unique curve  $\gamma : I \subset \mathbb{R} \rightarrow Q$  such that  $\gamma(0) = q$ ,  $\dot{\gamma}(0) = v$  and  $\ddot{\gamma}(t) = \Gamma(\gamma(t), \dot{\gamma}(t))$  (see [10] and references therein). Then we define  $\exp_{q,h}(v) = \gamma(h)$ . A natural idea to derive a numerical method is to consider a discretization of the exponential map  $\exp_{q,h}^d : U \subseteq T_qQ \rightarrow Q$  that is, an approximation of the continuous exponential map. If  $Q$  is a vector space, a common example of a discretization is the second order Taylor polynomial

$$\exp_{q,h}^d(v) = q + hv + \frac{h^2}{2}\Gamma(q, v). \tag{6}$$

**Definition 2.1.** A discretization of the exponential map of a second order differential equation is a family of maps  $\exp_{q,h}^d : T_qQ \rightarrow Q$  depending on a parameter  $h \in (-h_0, h_0)$  with  $h_0 > 0$  such that  $\exp_{q,0}^d(v) = q$ , that is, it is a constant map and the first and second derivatives with respect to  $h$  satisfy

$$\left. \frac{d}{dh} \right|_{h=0} \exp_{q,h}^d(v) = v, \quad \left. \frac{d^2}{dh^2} \right|_{h=0} \exp_{q,h}^d(v) = \Gamma(q, v).$$

**Definition 2.2.** The discrete flow  $\Phi_d^h : TQ \rightarrow TQ$ ,  $\Phi_d^h(q_k, v_k) = (q_{k+1}, v_{k+1})$  defined implicitly by the expression

$$\begin{cases} q_{k+1} = \exp_{q_k,h}^d(v_k) \\ q_k = \exp_{q_{k+1},-h}^d(v_{k+1}) \end{cases} \tag{7}$$

is called the *exponential method*.

Observe that by the implicit function theorem,  $\Phi_d^h$  is well-defined if  $T_v \exp_{q,h}^d$  is regular at  $v = v_{k+1}$  for any  $h \in (-h_0, h_0)$ . In other words,

$$\Phi_d^h(v_k) = \left[ \exp_{\exp_{q_k,h}^d(v_k),-h}^d \right]^{-1} (q_k), \quad \text{for } v_k \in T_{q_k}Q.$$

As we will see next, this is precisely the Newmark method with  $\beta = 0$  and  $\gamma = 1/2$ .

In general, we can recover any Newmark method as a map  $\Phi_d^h : TQ \rightarrow TQ$ ,  $\Phi_d^h(q_k, v_k) = (q_{k+1}, v_{k+1})$  using the following discretizations of the exponential map depending of a parameter  $\beta$  with  $0 \leq \beta \leq 1/2$ :

$$\exp_{q_k,h}^\beta(v_k) = q_k + hv_k + \frac{h^2}{2} ((1 - 2\beta)\Gamma(q_k, v_k) + 2\beta\Gamma(q_{k+1}, v_{k+1})) \tag{8}$$

and the Newmark method is rewritten as

$$\begin{cases} q_{k+1} = \exp_{q_k,h}^\beta(v_k) \\ q_k = \exp_{q_{k+1},-h}^{\beta'}(v_{k+1}) \end{cases} \tag{9}$$

with parameters  $0 \leq \beta, \beta' \leq 1/2$ . That is

$$\begin{aligned} q_{k+1} &= q_k + hv_k + \frac{h^2}{2}(1 - 2\beta)\Gamma(q_k, v_k) + h^2\beta\Gamma(q_{k+1}, v_{k+1}) \\ q_k &= q_{k+1} - hv_{k+1} + \frac{h^2}{2}(1 - 2\beta')\Gamma(q_{k+1}, v_{k+1}) + h^2\beta'\Gamma(q_k, v_k) \end{aligned} \tag{10}$$

Observe that these methods are equivalent to the Newmark methods with parameters  $\beta$  and  $\gamma = (1 + 2\beta' - 2\beta)/2$  in the expression (1) (in fact, if in (10) we put  $v_k = \dot{q}_k$  and  $v_{k+1} = \dot{q}_{k+1}$  then we obtain (1)).

**Remark 2.3.** The discretization of the exponential map given in Eq. (9) should be understood as follows. Given a discretization  $\Phi_d^h : TQ \rightarrow TQ$  of the flow of a second order differential equation then we can define the discretization of the exponential map as

$$\exp_{q_k,h}^\beta(v_k) = q_k + hv_k + \frac{h^2}{2} ((1 - 2\beta)\Gamma(q_k, v_k) + 2\beta\Gamma(\Phi_d^h(q_k, v_k))) .$$

Thus, it is clear that it only depends on the variables  $(q_k, v_k)$ .

### 3. The nonholonomic Newmark method

#### 3.1. Nonholonomic mechanics

Consider a nonholonomic system on the configuration space  $Q$  determined by a Lagrangian function  $L : TQ \rightarrow \mathbb{R}$  and nonholonomic constraints which are linear in the velocities given by a nonintegrable distribution  $\mathcal{D}$ . In coordinates,  $\mu_i^a(q) \dot{q}^i = 0$ ,  $m + 1 \leq a \leq n$ , where  $\text{rank}(\mathcal{D}) = m \leq n$ . The annihilator  $\mathcal{D}^\circ$  is locally given by  $\mathcal{D}^\circ = \{ \mu^a = \mu_i^a(q) dq^i; m + 1 \leq a \leq n \}$  where the 1-forms  $\mu^a$  are independent.

The equations of motion are completely determined by the Lagrange-d'Alembert principle [3]. This principle states that a curve  $q : [0, T] \rightarrow Q$  is an admissible motion of the system if

$$\delta \mathcal{J} = \delta \int_0^T L(q(t), \dot{q}(t)) dt = 0,$$

for all variations satisfying  $\delta q(t) \in \mathcal{D}_{q(t)}$ ,  $0 \leq t \leq T$ ,  $\delta q(0) = \delta q(T) = 0$ . The velocity of the curve itself must also satisfy the constraints, that is,  $\mu_i^a(q(t)) \dot{q}^i(t) = 0$ . From the Lagrange-d'Alembert principle, we arrive at the well-known **nonholonomic equations**

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} = \lambda_a \mu_i^a, \tag{11a}$$

$$\mu_i^a(q) \dot{q}^i = 0, \tag{11b}$$

where  $\lambda_a$ ,  $m + 1 \leq a \leq n$ , is a set of Lagrange multipliers to be determined. The right-hand side of Eq. (11a) represents the force induced by the constraints (reaction forces), while Eq. (11b) gives the linear velocity constraint condition.

If we assume that the nonholonomic system is regular (see [11]), which is guaranteed if the Hessian matrix  $(W_{ij}) = \left( \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} \right)$  is positive (or negative) definite, then the nonholonomic equations can be characterized as the solutions of a second order differential equation  $\Gamma_{nh}$  restricted to the constraint space determined by  $\mathcal{D}$ . We can rewrite Eq. (11a) as a vector field on the tangent bundle  $\Gamma_{nh} = \Gamma_L + \lambda_a Z^a$  where

$$\Gamma_L = \dot{q}^i \frac{\partial}{\partial q^i} + W^{ij} \left( \frac{\partial L}{\partial q^j} - \frac{\partial^2 L}{\partial \dot{q}^i \partial q^k} \dot{q}^k \right) \frac{\partial}{\partial \dot{q}^i}, \quad Z^a = W^{ij} \mu_j^a \frac{\partial}{\partial \dot{q}^i}$$

where  $(W^{ij})$  is the inverse matrix of  $(W_{ij})$  (see [11,12]). Moreover, the Lagrange multipliers are completely determined and are given by the expression  $\lambda_a = -C_{ab} \Gamma_L(\mu_i^b \dot{q}^i)$ , where  $(C_{ab})$  is the inverse matrix of  $(C^{ab}) = (\mu_j^a W^{ij} \mu_i^b)$ . This matrix is invertible if and only if the nonholonomic system  $(L, \mathcal{D})$  is regular.

#### 3.2. Numerical methods for nonholonomic systems

There have been several attempts to capture the nature of nonholonomic mechanics in the discrete setting (cf. [5,6,13–20]). The literature is far too vast on this topic and our purpose is not to make a detailed comparison between the different methods (see [4] for an excellent comparison) but rather describing the advantages and disadvantages of using each method in order to introduce better the advantages of considering the method we propose in this paper.

In the following, we will restrict to the case where the mechanical system is defined by a Lagrangian function  $L : T\mathbb{R}^n \rightarrow \mathbb{R}$  of the form  $L(q, \dot{q}) = \frac{1}{2} \dot{q}^T M \dot{q} - V(q)$ , where  $M$  is a constant mass matrix and consider the nonholonomic constraints given by a rank  $k$  distribution  $\mathcal{D}$  defined by the matrix equation  $\mu(q)\dot{q} = 0$  where  $\mu(q)$  is a  $m \times n$  matrix for each  $q$  and  $m = n - k$ .

The nonholonomic leap-frog method [5,6] is given by the algorithm

$$\begin{cases} q_{k+1} = q_k + h\dot{q}_k - \frac{h^2}{2} M^{-1}(\nabla V(q_k) + \mu^T(q_k)\tilde{\lambda}_k) \\ \dot{q}_{k+1} = \dot{q}_k - \frac{h}{2} M^{-1}(\nabla V(q_k) + \mu^T(q_k)\tilde{\lambda}_k + \nabla V(q_{k+1}) + \mu^T(q_{k+1})\tilde{\lambda}_{k+1}) \\ \mu(q_k)\dot{q}_k = 0 \\ \mu(q_{k+1})\dot{q}_{k+1} = 0. \end{cases}$$

and generates a discrete flow of the type  $(q_k, \dot{q}_k, \tilde{\lambda}_k) \mapsto (q_{k+1}, \dot{q}_{k+1}, \tilde{\lambda}_{k+1})$ .

The DLA method proposed in [15] with a midpoint discretization  $\alpha = 1/2$  may be written in the following form:

$$\begin{cases} q_{k+1} = q_k + h\dot{q}_k - \frac{h^2}{4} M^{-1}(\nabla V(q_k) + \nabla V(q_{k+1})) + \frac{h^2}{2} \mu^T(q_k + \frac{h}{2}\dot{q}_k)\lambda \\ \dot{q}_{k+1} = \dot{q}_k - \frac{h}{2} M^{-1}(\nabla V(q_k) + \nabla V(q_{k+1})) + h\mu^T(q_k + \frac{h}{2}\dot{q}_k)\lambda \\ \mu(q_k)\dot{q}_k = 0 \\ \mu(q_{k+1})\dot{q}_{k+1} = 0. \end{cases}$$

In Sections 5 and 6 of [2], the authors proposed a Newmark method for general nonholonomic mechanics. In particular, for  $\alpha_m = \alpha_f = 0$  (using their notation) they derive the following integrator:

$$\begin{cases} q_{k+1} = q_k + h\dot{q}_k + \frac{h^2}{2} ((1 - 2\beta)\Gamma_{nh}(q_k, \dot{q}_k, \lambda_k) + 2\beta\Gamma_{nh}(q_{k+1}, \dot{q}_{k+1}, \lambda_{k+1})) \\ \dot{q}_{k+1} = \dot{q}_k + h((1 - \gamma)\Gamma_{nh}(q_k, \dot{q}_k, \lambda_k) + \gamma\Gamma_{nh}(q_{k+1}, \dot{q}_{k+1}, \lambda_{k+1})) \\ \phi^a(q_{k+1}, \dot{q}_{k+1}) = 0. \end{cases} \tag{12}$$

where they choose as initial value of the Lagrange multiplier the continuous one, that is,  $\lambda_0 = -C_{ab}(q_0, \dot{q}_0)\Gamma_L(\mu_i^b \dot{q}^i) \Big|_{(q_0, \dot{q}_0)}$ . Observe that, in the particular case of a nonholonomic system given by a Lagrangian of the type (2) and constraints determined by a distribution  $\mathcal{D}$  and choosing the parameters  $\beta = 0$  and  $\gamma = 1/2$  we exactly obtain the nonholonomic leap-frog method.

### 3.3. The discrete constraint space for nonholonomic systems

Given a nonholonomic system  $(L, \mathcal{D})$ , the *nonholonomic exponential map* at  $q \in Q$  and at time  $h > 0$  is the map

$$\text{exp}_{q,h}^{nh} : \mathcal{U}_q \subseteq \mathcal{D}_q \longrightarrow Q, \quad v_q \mapsto c_{v_q}^{nh}(h)$$

sending each tangent vector  $v_q$  in the distribution to the unique nonholonomic trajectory starting at  $q$  with initial velocity  $v_q$  evaluated at time  $h$  (see [21] for more details; see also [22]).

The fact that the space of initial velocities is restricted to the subspace  $\mathcal{D}_q$ , implies that the set of points reached by nonholonomic trajectories starting at  $q$ , that is, the image of  $\text{exp}_{q,h}^{nh}$  is a submanifold of  $Q$ . Thus, we define the *exact discrete constraint space* at  $q$  as

$$\mathcal{M}_{q,h}^{nh} := \text{exp}_{q,h}^{nh}(\mathcal{D}_q). \tag{13}$$

We are intentionally committing a slight abuse of notation in the definition of  $\mathcal{M}_{q,h}^{nh}$ , since not all vectors in  $\mathcal{D}_q$  are guaranteed to generate a nonholonomic trajectory defined up to time  $h$ . But if  $h$  is sufficiently small, we can always consider a non-empty open subset of  $\mathcal{D}_q$  generating such well-defined trajectories.

Moreover, it can be proven that  $\text{exp}_{q,h}^{nh}$  is a diffeomorphism from an open subset  $\mathcal{U}_q$  in  $\mathcal{D}_q$  to  $\mathcal{M}_{q,h}^{nh}$ . Thus, in particular, the dimension of  $\mathcal{M}_{q,h}^{nh}$  is precisely  $\text{rank}(\mathcal{D})$  (see [21,22]).

This observation is particularly important, since it shows that if  $q_1$  and  $q_0$  are two sufficiently close points connected by a nonholonomic trajectory, then  $q_1$  is restricted to live in the submanifold  $\mathcal{M}_{q_0,h}^{nh}$  with strictly lower dimension than  $Q$  (in fact  $\dim \mathcal{M}_{q_0,h}^{nh} = m$ ). We will take this restriction into account when constructing numerical methods for nonholonomic systems. Though this procedure mimics the exact situation, we are also introducing a new source of error in the numerical integrator, since the discrete space must be approximated.

Assume that we have a nonholonomic system given by  $(L, \mathcal{D})$  with nonholonomic dynamics given by  $\Gamma_{nh}(q, v, \lambda) = \Gamma_L(q, v) + \lambda Z(q, v)$  and the Lagrange multipliers are derived from the nonholonomic constraints  $\dot{c}(t) \in \mathcal{D}_{c(t)}$ .

The equations of motion of a nonholonomic system are completely determined by the nonholonomic exponential map. In fact the unique solution  $\gamma : I \subset \mathbb{R} \rightarrow Q$  of the constrained SODE  $\Gamma_{nh}$  with initial condition such that  $\gamma(0) = q$ ,  $\dot{\gamma}(0) = v_q \in \mathcal{D}_q$  is characterized by  $\gamma(h) = \text{exp}_{q,h}^{nh}(v_q)$ . From the properties of vector field flows, in this case  $\Gamma_{nh}$ , we have the following compatibility conditions  $\text{exp}_{q,h}^{nh}(v_q) = \text{exp}_{\tilde{q},(s-1)h}^{nh}(\tilde{v}_{\tilde{q}})$  where  $\tilde{q} = \gamma(h) = \text{exp}_{q,h}^{nh}(v_q)$ ,  $\tilde{v}_{\tilde{q}} = \dot{\gamma}(h)$  and  $s \in [0, 1]$ . In particular, for  $s = 0$  and  $s = 1$ , we obtain the following system of equations

$$\tilde{q} = \text{exp}_{q,h}^{nh}(v_q), \quad q = \text{exp}_{\tilde{q},-h}^{nh}(\tilde{v}_{\tilde{q}}). \tag{14}$$

Observe that the final position and velocity satisfy the constraints  $\tilde{q} \in \mathcal{M}_{q,h}^{nh}$  and  $\tilde{v}_{\tilde{q}} \in \mathcal{D}_{\tilde{q}}$ .

### 3.4. The nonholonomic Newmark method

Following Eqs. (14), we will impose some constraints in order to obtain a nonholonomic version of the Newmark method:  $(q_k, v_k) \rightarrow (q_{k+1}, v_{k+1})$ . In particular, we need an appropriate discretization

$$\text{exp}_{q,h}^{d,\beta,\lambda,\lambda'} : \mathcal{D}_q \rightarrow Q$$

of the nonholonomic exponential map depending on a parameter  $0 \leq \beta \leq 1/2$  and Lagrange multipliers  $\lambda$  and  $\lambda'$  which force the final point to satisfy a discretization of the exact discrete constraint space, denoted by  $\mathcal{M}_{q_k,h}^d \subseteq Q$ , with  $\dim \mathcal{M}_{q_k,h}^d = \text{rank}(\mathcal{D})$ , and the final velocity to belong to  $\mathcal{D}$ . More concretely, we have the following definition

$$\text{exp}_{q_k,h}^{d,\beta,\lambda,\lambda'}(v_k) = q_k + hv_k + \frac{h^2}{2} ((1 - 2\beta)\Gamma_{nh}(q_k, v_k, \lambda_k) + 2\beta\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1}))$$

where we are denoting the second component  $\Gamma_{nh}(q, v, \lambda) = \Gamma_L(q, v) + \lambda Z(q, v)$  of the vector field  $\Gamma_{nh}$  with the same letter to avoid overloading notation. Therefore, our proposal of nonholonomic Newmark method is:

**Definition 3.1.** The **nonholonomic Newmark method** with parameters  $(\beta, \beta')$ ,  $0 \leq \beta, \beta' \leq 1/2$  is the integrator  $F_h^{\beta, \beta'} : \mathcal{D} \rightarrow \mathcal{D}$  implicitly given by

$$\begin{aligned} q_{k+1} &= \exp_{q_k, h}^{d, \beta, \lambda, \lambda'}(v_k) \\ q_k &= \exp_{q_{k+1}, -h}^{d, \beta', \lambda', \lambda}(v_{k+1}) \\ q_{k+1} &\in \mathcal{M}_{q_k, h}^d \\ v_{k+1} &\in \mathcal{D}_{q_{k+1}}, \end{aligned}$$

or

$$\begin{cases} q_{k+1} = q_k + hv_k + \frac{h^2}{2} \left( (1 - 2\beta)\Gamma_{nh}(q_k, v_k, \lambda_k) + 2\beta\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1}) \right) \\ q_k = q_{k+1} - hv_{k+1} + \frac{h^2}{2} \left( 2\beta'\Gamma_{nh}(q_k, v_k, \lambda_k) + (1 - 2\beta')\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1}) \right) \\ q_{k+1} \in \mathcal{M}_{q_k, h}^d \\ v_{k+1} \in \mathcal{D}_{q_{k+1}}. \end{cases}$$

If the constraint distribution is given as the zero set of the functions  $\phi^a : TQ \rightarrow \mathbb{R}$ , i.e.,  $\phi^a(q_k, v_k) = 0$  and the discrete constraint space is given as the zero set of the functions  $\Phi^a : Q \times Q \rightarrow \mathbb{R}$ , i.e.,  $\Phi^a(q_k, q_{k+1}) = 0$ , then the discrete equations can be written as

$$\begin{cases} q_{k+1} = q_k + hv_k + \frac{h^2}{2} \left( (1 - 2\beta)\Gamma_{nh}(q_k, v_k, \lambda_k) + 2\beta\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1}) \right) \\ q_k = q_{k+1} - hv_{k+1} + \frac{h^2}{2} \left( 2\beta'\Gamma_{nh}(q_k, v_k, \lambda_k) + (1 - 2\beta')\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1}) \right) \\ \Phi^a(q_k, q_{k+1}) = 0 \\ \phi^a(q_{k+1}, v_{k+1}) = 0. \end{cases}$$

**Remark 3.2.** In the case of holonomic constraints, that is, when the distribution  $\mathcal{D}$  is integrable, the exact discrete constraint space  $\mathcal{M}_{q_k, h}^{nh}$  is precisely the leaf  $\mathcal{L}_{q_k}$  of the foliation by the point  $q_k$  integrating the distribution and the constraint distribution is just the tangent space to each leaf (see [21,22]). Therefore, the nonholonomic Newmark method in the holonomic case becomes (see [23]):

$$\begin{cases} q_{k+1} = q_k + hv_k + \frac{h^2}{2} \left( (1 - 2\beta)\Gamma_{nh}(q_k, v_k, \lambda_k) + 2\beta\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1}) \right) \\ q_k = q_{k+1} - hv_{k+1} + \frac{h^2}{2} \left( 2\beta'\Gamma_{nh}(q_k, v_k, \lambda_k) + (1 - 2\beta')\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1}) \right) \\ q_{k+1} \in \mathcal{L}_{q_k} \\ v_{k+1} \in \mathcal{D}_{q_{k+1}}. \end{cases}$$

**Remark 3.3.** A very important caveat is that when  $\beta + \beta' = 1/2$ , the system of equations given by the nonholonomic Newmark method becomes ill-conditioned, at least for the case of mechanical Lagrangians. This is because the Jacobian matrix of the system with respect to the unknowns  $(q_{k+1}, v_{k+1}, \lambda_k, \lambda'_{k+1})$  has two columns, those corresponding to the Lagrange multipliers, that are almost proportional. Each numerical step gives results with a large uncertainty, which accumulates rapidly. Therefore, this choice of parameters, which of course includes the case  $\beta = \beta' = 1/4$ , should be avoided.

**Remark 3.4.** The Newmark method (12) proposed by [2] is of a different nature than our proposal of nonholonomic Newmark method since we do not need an initial value of the Lagrange multiplier and we also add a discrete version of the nonholonomic constraint, in addition to the continuous nonholonomic constraint.

### 3.5. Discretizations of the exact discrete constraint space

Suppose that the nonholonomic constraints defining the distribution  $\mathcal{D}$ , as a submanifold of  $TQ$ , are  $\phi^a(q, v) = \langle \mu^a(q), v \rangle$  and, additionally, that the discrete constraints are obtained from the continuous ones in the following way

$$\Phi^a(q_k, q_{k+1}) = \left\langle \mu^a \left( (1 - \alpha)q_k + \alpha q_{k+1} \right), \frac{q_{k+1} - q_k}{h} \right\rangle, \quad \alpha \in [0, 1]. \tag{15}$$

Alternatively, it would be also possible to consider

$$\tilde{\Phi}^a(q_k, q_{k+1}) = \left\langle (1 - \alpha)\mu^a(q_k) + \alpha\mu^a(q_{k+1}), \frac{q_{k+1} - q_k}{h} \right\rangle, \quad \alpha \in [0, 1]. \tag{16}$$

Whenever it is clear which of the constraint discretizations we are using, we will simply denote the associated nonholonomic Newmark flow by  $F_h^{\beta, \beta', \alpha} : \mathcal{D} \rightarrow \mathcal{D}$ .

In this sense, let  $\mathcal{M}_{q_k, h}^d \subseteq Q$  for each  $q_k \in Q$  be the submanifold  $\mathcal{M}_{q_k, h}^d = \{q_{k+1} \mid \Phi^a(q_k, q_{k+1}) = 0\}$ .

For deriving nonholonomic Newmark methods of order two, it would be interesting to assume the following **symmetry condition** in the discretization of the exact discrete constraint space:

$$q_{k+1} \in \mathcal{M}_{q_k, h}^d \Leftrightarrow q_k \in \mathcal{M}_{q_{k+1}, h}^d$$

For instance, this condition is satisfied if  $\alpha = 1/2$  in the discretizations given by (15) and (16).

As a direct consequence using the symmetry of the method we obtain the following proposition (see [24]).

**Proposition 3.5.** *The nonholonomic Newmark methods with  $\beta = \beta'$  and a symmetric discretization of the constraints are at least of order 2.*

Thus, the nonholonomic Newmark method  $F_h^{\beta, \beta, 1/2} : \mathcal{D} \rightarrow \mathcal{D}$  associated to either discretizations is at least of order 2.

### 3.6. Some interesting cases of nonholonomic Newmark methods

The following result shows that, in some particular cases, the nonholonomic Newmark method corresponds with the DLA algorithm, one of the most classical geometric integrators for nonholonomic systems (see [15]).

**Proposition 3.6.** *Assume that we have a nonholonomic system defined by a Lagrangian of the type (2) and a distribution  $\mathcal{D}$ . For any  $\alpha \in [0, 1]$  and for  $\beta = \beta' = 0$ , the nonholonomic Newmark method  $F_h^{0, 0, \alpha} : \mathcal{D} \rightarrow \mathcal{D}$  is equivalent to the DLA algorithm with discrete Lagrangian given by*

$$\begin{aligned} L_d^{sym, \alpha}(q_k, q_{k+1}) &= h \left[ (1 - \alpha)L \left( q_k, \frac{q_{k+1} - q_k}{h} \right) + \alpha L \left( q_{k+1}, \frac{q_{k+1} - q_k}{h} \right) \right] \\ &= h \left( \frac{q_{k+1} - q_k}{h} \right) M \left( \frac{q_{k+1} - q_k}{h} \right)^T - h(1 - \alpha)V(q_k) - h\alpha V(q_{k+1}) \end{aligned} \tag{17}$$

for each  $\alpha$  and using either discretization (15) or (16).

**Proof.** In this particular case

$$\Gamma_L(q_k, v_k) = -M^{-1}\nabla V(q_k) \text{ and } Z^a(q_k) = M^{-1}\mu^a(q_k)$$

From the equations of the nonholonomic Newmark method we obtain

$$\begin{aligned} q_k &= q_{k+1} - hv_{k+1} + \frac{h^2}{2}\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1}) \\ q_{k+2} &= q_{k+1} + hv_{k+1} + \frac{h^2}{2}\Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda_{k+1}) \end{aligned}$$

adding both equations we immediately deduce that

$$\frac{q_{k+2} - 2q_{k+1} + q_k}{h^2} = \Gamma_L(q_{k+1}, v_{k+1}) + \frac{\lambda_{k+1} + \lambda'_{k+1}}{2}Z(q_{k+1}).$$

or equivalently,

$$\frac{q_{k+2} - 2q_{k+1} + q_k}{h^2} = -M^{-1}\nabla V(q_{k+1}) + \frac{\lambda_{k+1} + \lambda'_{k+1}}{2}M^{-1}\mu(q_{k+1}).$$

These equations are equivalent to the DLA integrator with respect to the discrete Lagrangian  $L_d^{sym, \alpha}(q_k, q_{k+1})$  and the constraints (15): with the relation between Lagrange multipliers being  $\Lambda = \frac{h(\lambda_{k+1} + \lambda'_{k+1})}{2}$ , where  $\Lambda$  is the Lagrange multiplier appearing in the DLA method [15].  $\square$

Moreover, using the previous method, we can produce new numerical integrators using composition and the adjoint method (see [24], Chapter II.3). If  $\Phi_h$  is a numerical method then the adjoint method is given by  $\Phi_h^* = (\Phi_{-h})^{-1}$ . An example of composition of numerical methods is shown in the next Proposition:

**Proposition 3.7.** *Consider the nonholonomic Newmark method with  $\beta = \beta' = 0$  and  $\alpha = 0$  denoted by  $F_h^{0, 0, 0}$ , and its adjoint method  $(F_h^{0, 0, 0})^*$ . The composition of these two methods*

$$\Psi_h = (F_{h/2}^{0, 0, 0})^* \circ F_{h/2}^{0, 0, 0} \tag{18}$$

generates a second order method, using standard results on composition of adjoint methods.

**Proof.** The last result holds directly from the results in [24].  $\square$



But we can say more, we may prove that  $(F_h^{0,0,0})^* = F_h^{0,0,1}$  and obtain:

**Proposition 3.8.** *Let  $\beta = \beta' = 0$ . The nonholonomic Newmark methods with  $\alpha = 0, 1$ , denoted by  $F_h^{0,0,0}$  and  $F_h^{0,0,1}$ , respectively, are adjoint methods. Therefore, the composition of these two methods*

$$\Psi_h = F_{h/2}^{0,0,1} \circ F_{h/2}^{0,0,0} \tag{19}$$

generates a second order method, using standard results on composition of adjoint methods.

**Proof.** Observe that the method  $F_h^{0,0,0}$  is given by the equations

$$\begin{aligned} q_{k+1} &= q_k + hv_k + \frac{h^2}{2} \Gamma_{nh}(q_k, v_k, \lambda_k) \\ q_k &= q_{k+1} - hv_{k+1} + \frac{h^2}{2} \Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1}) \\ v_{k+1} &\in \mathcal{D}_{q_{k+1}} \\ 0 &= \langle \mu^a(q_k), \frac{q_{k+1} - q_k}{h} \rangle \end{aligned}$$

It is a straightforward verification that its adjoint method  $(F_h^{0,0,0})^*$  is given by the same equations except that the last one becomes  $0 = \langle \mu^a(q_{k+1}), \frac{q_{k+1} - q_k}{h} \rangle$ . This means that  $(F_h^{0,0,0})^* = F_h^{0,0,1}$  and the result follows.  $\square$

Consider the Newmark methods with  $\beta = \beta' = 0$  and a Lagrangian of the type  $L(q, \dot{q}) = \frac{1}{2} \dot{q} M \dot{q}^T - V(q)$ . Suppose that we discretize the constraint space using the parameter  $\alpha = 0$ , i.e.,

$$\mathcal{M}_{q_k, h}^d = \left\{ q_{k+1} \mid \left\langle \mu^a(q_k), \frac{q_{k+1} - q_k}{h} \right\rangle = 0 \right\}.$$

Then from the equation  $q_{k+1} = q_k + hv_k + \frac{h^2}{2} \Gamma_{nh}(q_k, v_k, \lambda_k)$ , we explicitly obtain the Lagrange multiplier  $\lambda_k$ :

$$\lambda_k = \frac{\langle \mu(q_k), M^{-1} \nabla V(q_k) \rangle}{\| \mu(q_k) \|_M^2}$$

where  $\| \mu(q_k) \|_M = \sqrt{\mu_i^a(q_k) M^{ij} \mu_j^b(q_k)}$ . In consequence we explicitly derive  $q_{k+1}$  as

$$q_{k+1} = q_k + hv_k + \frac{h^2}{2} \left( -M^{-1} \nabla V(q_k) + \frac{\langle \mu(q_k), M^{-1} \nabla V(q_k) \rangle}{\| \mu(q_k) \|_M^2} M^{-1} \mu(q_k) \right)$$

Then, applying the co-vector  $\mu(q_{k+1})$  to the second equation

$$q_k = q_{k+1} - hv_{k+1} + \frac{h^2}{2} \Gamma_{nh}(q_{k+1}, v_{k+1}, \lambda'_{k+1})$$

we obtain

$$\lambda'_{k+1} = -\frac{2}{h \| \mu(q_{k+1}) \|_M^2} \left\langle \mu(q_{k+1}), \frac{q_{k+1} - q_k}{h} \right\rangle + \frac{\langle \mu(q_{k+1}), M^{-1} \nabla V(q_{k+1}) \rangle}{\| \mu(q_{k+1}) \|_M^2}$$

and in consequence we also derive explicitly  $v_{k+1}$ .

**Proposition 3.9.** *The nonholonomic Newmark method  $F_h^{0,0,0} : \mathcal{D} \rightarrow \mathcal{D}$  is completely explicit for Lagrangians of the type (2) and constraints of the type  $\alpha = 0$ .*

**Remark 3.10.** In fact, Proposition 3.9 is more general and can be trivially generalized for Lagrangians of mechanical type  $L(q, \dot{q}) = \frac{1}{2} \dot{q} M(q) \dot{q}^T - V(q)$ , where  $M(q)$  is a positive definite matrix for all  $q \in Q$ .

**Remark 3.11.** The Newmark method  $F_h^{0,0,0}$  is related to the nonholonomic leap-frog method though they are of a very different nature. The main difference (see Remark 3.4) between both of them is the existence of an additional discrete constraint in the nonholonomic Newmark method. This difference has practical consequences on the nature of the flow. With an additional equation, the value of the Lagrange multiplier's is now completely determined by the imposition of the discrete constraints and the algorithm evolves on  $\mathcal{D}$ . However, in the nonholonomic leap-frog method, the absence of the discrete constraints implies that the Lagrange multiplier will behave like an extra variable and the method will evolve on  $\mathcal{D} \times \mathbb{R}^m$ . In practice, this means we must choose an initial Lagrange multiplier to initialize the algorithm.

Now, the nonholonomic Newmark method does include Lagrange multipliers but they are not treated as a variable: they are determined by the constraints and do not need to be given an initial value. In other words, the Lagrange



multipliers are functions of the state variables. As we have seen above, for the Newmark method  $F_h^{0,0,0}$ , the expression of the multipliers is computed explicitly and if we take its value as the initial Lagrange multiplier in the nonholonomic leap-frog method, we will obtain the same updates on positions and velocities. However, the flow cannot be considered the same because the nonholonomic leap-frog method also provides an update in the multipliers that is needed in order to compute the next iteration. In general, it has no relation with the multipliers appearing in the Newmark method.

**Remark 3.12.** We have introduced in Sections 3.4 and 3.5 first and second-order nonholonomic Newmark methods depending on the concrete values  $(\beta, \beta')$  and the discretization of the exact discrete constraint space. As we have seen in Propositions 3.7 and 3.8 we can design new methods preserving the nonholonomic constraints using the idea of composing methods. In the same way, we can produce higher-order nonholonomic integrators using nonholonomic Newmark methods as building blocks (see [24–26]).

For instance, considering the second-order nonholonomic Newmark method  $F_h^{0,0,1/2} : \mathcal{D} \rightarrow \mathcal{D}$  and using the triple jump [24], we obtain a fourth order method  $\Psi_h : \mathcal{D} \rightarrow \mathcal{D}$  given by:  $\Psi_h = F_{\gamma_1 h}^{0,0,1/2} \circ F_{\gamma_2 h}^{0,0,1/2} \circ F_{\gamma_1 h}^{0,0,1/2}$  where

$$\gamma_1 = \frac{1}{2 - 2^{1/3}}, \quad \gamma_2 = -\frac{2^{1/3}}{(2 - 2^{1/3})}.$$

Using similar constructions, we can derive higher-order methods for nonholonomic mechanics with order 6, 8, etc. Thus, other choices of the parameters produce different higher-order numerical methods (see, for instance, [27]).

### 4. Examples of nonholonomic systems

#### 4.1. Chaotic nonholonomic particle

In this example, we study a particle moving on the configuration space  $Q = \mathbb{R}^5$  with coordinates  $q = (x, y_1, y_2, z_1, z_2)$  and described by the mechanical Lagrangian function [6]:

$$L(q, \dot{q}) = \frac{1}{2} \|\dot{q}\|^2 - \frac{1}{2} (\|q\|^2 + z_1^2 z_2^2 + y_1^2 z_1^2 + y_2^2 z_2^2),$$

where  $\|\cdot\|$  denotes the euclidean norm, and subjected to the single constraint  $\dot{x} + y_1 \dot{z}_1 + y_2 \dot{z}_2 = 0$  (see [6]).

The motion of the chaotic particle is given by the system of differential equations

$$\begin{cases} \ddot{x} = -x + \lambda, & \ddot{y}_1 = -y_1 - y_1 z_1^2, \\ \ddot{y}_2 = -y_2 - y_2 z_2^2, & \ddot{z}_1 = -z_1 - z_1 z_2^2 - y_1^2 z_1 + \lambda y_1, \\ \ddot{z}_2 = -z_2 - z_1^2 z_2 - y_2^2 z_2 + \lambda y_2, & \dot{x} + y_1 \dot{z}_1 + y_2 \dot{z}_2 = 0. \end{cases}$$

#### 4.2. Pendulum-driven CVT system

This example in  $Q = \mathbb{R}^3$  is a nonholonomic continuous variable transmission (CVT) system determined by an independent Hamiltonian subsystem called the driver system [4]. We will denote the coordinates in  $\mathbb{R}^3$  by  $(x, y, \xi)$  and, then, the Lagrangian function is

$$L(x, y, \xi, \dot{x}, \dot{y}, \dot{\xi}) = \frac{1}{2} \left( \sum_{i=1}^2 \dot{q}_i^2 + \kappa_i q_i^2 \right) + l(\xi, \dot{\xi}),$$

where  $(q_1, q_2, \dot{q}_1, \dot{q}_2) = (x, y, \dot{x}, \dot{y})$  and  $l(\xi, \dot{\xi}) = \frac{1}{2} \dot{\xi}^2 - V(\xi)$  is called the *driver energy*, while the first term depending only on  $q_i$  and  $\dot{q}_i$  is called the *passenger energy*. The nonholonomic constraint is of the form  $\dot{y} + f(\xi)\dot{x} = 0$ .

The motion of this family of systems is given by the equations

$$\begin{cases} \ddot{x} = \kappa_1 x + \lambda f(\xi) & \ddot{y} = \kappa_2 y + \lambda \\ \ddot{\xi} = -V'(\xi) & \dot{y} + f(\xi)\dot{x} = 0 \end{cases}$$

where the Lagrange multiplier may be computed to be of the form

$$\lambda = -\frac{f'(\xi)\dot{\xi}\dot{x} + \kappa_1 f(\xi)x + \kappa_2 y}{1 + f^2(\xi)}.$$

From now on, consider the following potential and constraint functions and constants

$$V(\xi) = \cos(\xi) - \frac{\epsilon \sin(2\xi)}{2}, \quad f(\xi) = \sin(\xi), \quad \kappa_1 = \kappa_2 = -1.$$

This example has the property that for  $\epsilon \neq 0$ , the system is no longer integrable reversible and so, good long time behaviour observed in most nonholonomic integrators is lost in this case (see [4]).

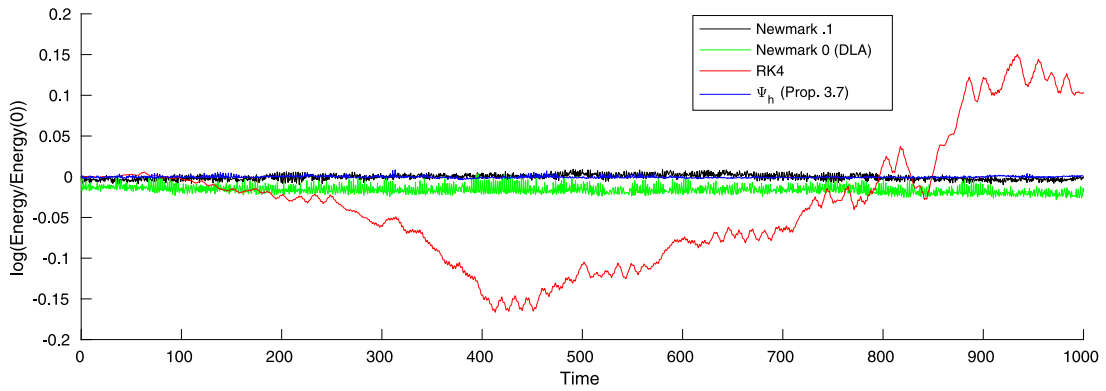


Fig. 1. Energy drift for the chaotic nonholonomic particle.

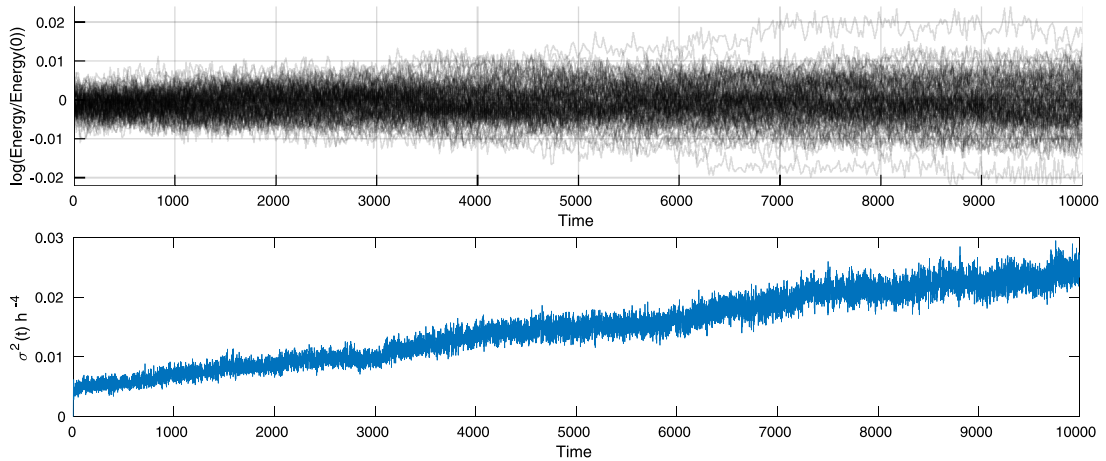


Fig. 2. Energy drift and variance for 100 random trajectories of the chaotic nonholonomic particle, with  $\beta = \beta' = .1$ .

## 5. Numerical results

### 5.1. Chaotic nonholonomic particle

Fig. 1 shows the energy drift for the nonholonomic Newmark method with  $\beta = \beta' = 0$  (DLA), the nonholonomic Newmark method with  $\beta = \beta' = .1$ , both with  $\alpha = 1/2$ , a Runge–Kutta 4th order method and the composition method  $\Psi_h$  in Proposition 3.8. Here we used  $T = 1000$ ,  $h = .2$ , and initial conditions  $q_0 = (1, 0, 1, -1, -1)$ ,  $v_0 = (0.05, 0.5, -0.5, -0.1, -0.05)$ , with energy 3.2575 approximately.

For this example, the methods we propose here outperform Runge–Kutta in energy behaviour.

We also explore 100 random initial conditions for this example, all of them having the same energy value of 1.535. We used  $\beta = \beta' = .1$ ,  $T = 10000$  and  $h = .2$ . The method used is the composition method in Proposition 3.8. In Fig. 2 we plot the energy drift for each trajectory and the variance of the energy drift as in [6].

### 5.2. Pendulum-driven CVT

We first consider the case  $\epsilon = 0$ . In Fig. 3 we show the energy drift for the nonholonomic Newmark method with  $\beta = \beta' = 0$ , and with  $\beta = \beta' = .1$ , both with  $\alpha = 1/2$ , 4th-order Runge–Kutta, and the composition method  $\Psi_h$ . Here  $T = 400$ ,  $h = .2$ , and the initial conditions are  $q_0 = (1, 0, -2)$ ,  $v_0 \approx (-0.4481, -0.4075, 0.1)$ , with an approximate energy of 0.2723.

For the case  $\epsilon = 0.1$  in Fig. 4, we compare the nonholonomic Newmark method with  $\beta = \beta' = 0$ ,  $\alpha = 1/2$ , and the nonholonomic Leap-Frog method as well as the composition methods  $\Psi_h$  and  $\Psi_{2h}$ . The latter was included because the computational cost for each step of  $\Psi_h$  is twice that of the nonholonomic Newmark method; therefore  $\Psi_{2h}$  has a global computational cost comparable to the nonholonomic Newmark method. Here  $h = .05$ ,  $T = 7500$ , and the initial

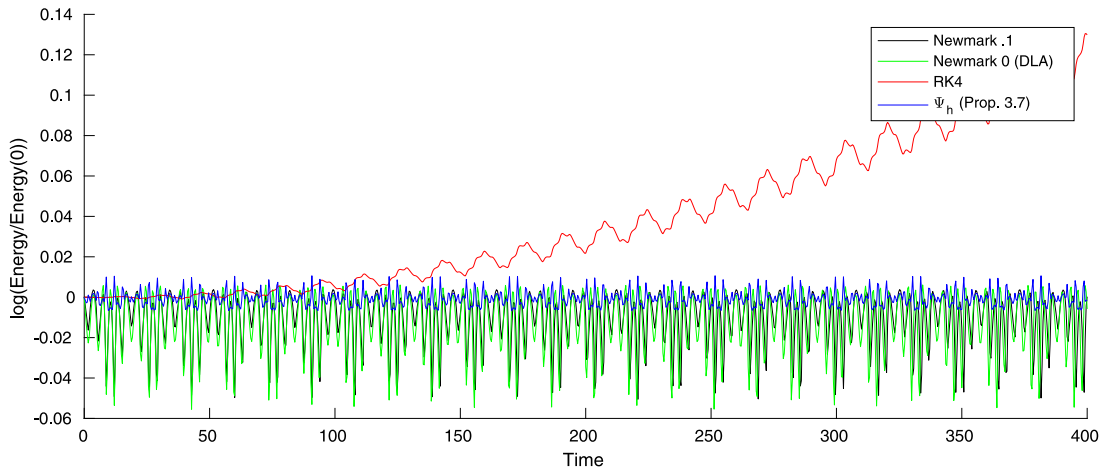


Fig. 3. Energy drift for the pendulum-driven CVT,  $\epsilon = 0$ .

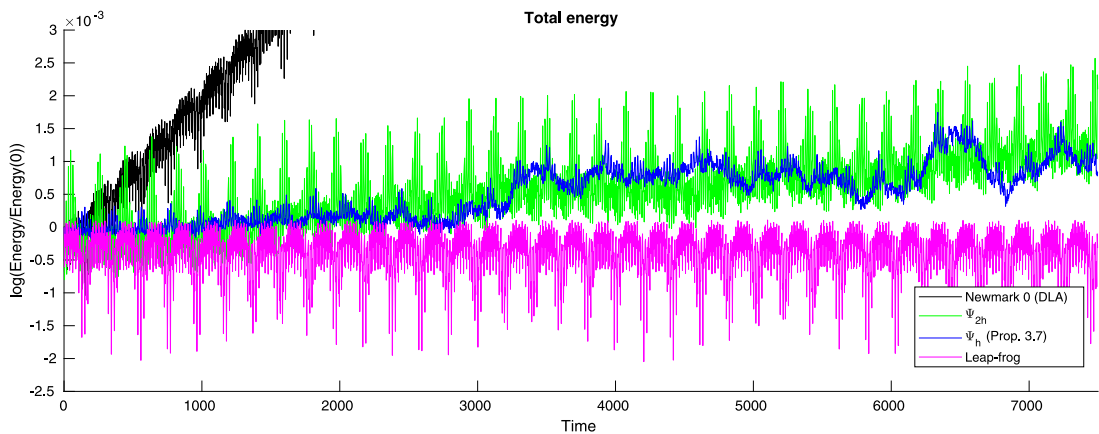


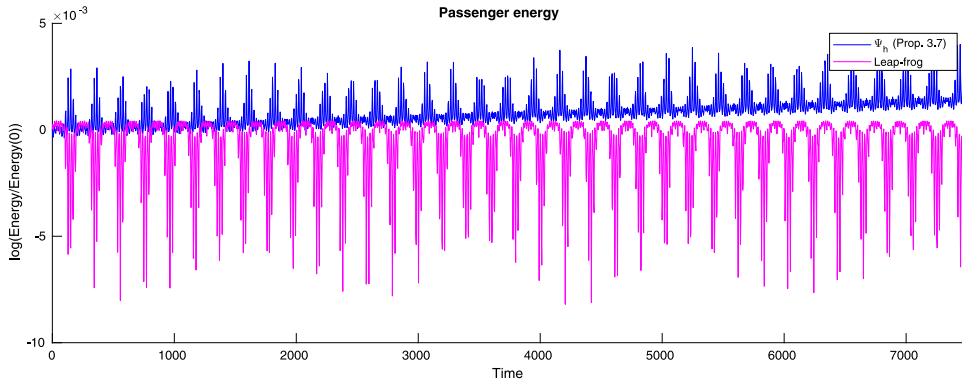
Fig. 4. Total energy for the pendulum-driven CVT,  $\epsilon = 0.1$ . Newmark 0 truncated in order to show details of the other methods.

conditions are the same as the ones used in [4], which are  $q_0 = (1, 1, 0)$ ,  $v_0 \approx (0, 0, 2.82842712)$ , now the energy being exactly 6.0.

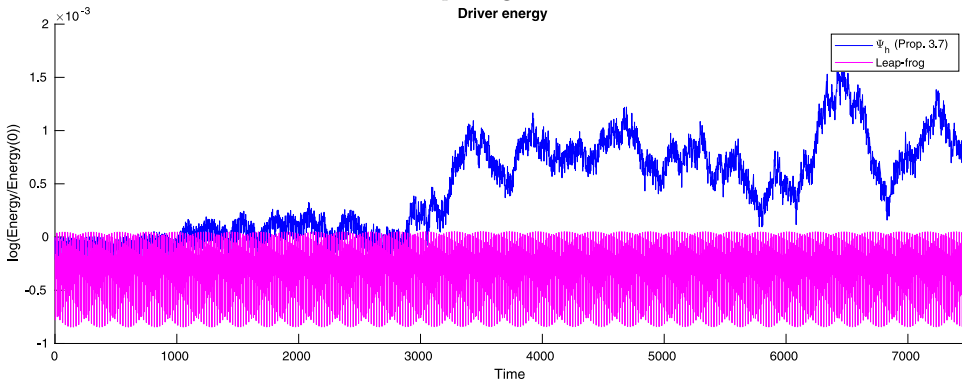
As expected, we observe that the Newmark method, being equivalent to the DLA method, is no longer able to preserve energy as it had been already pointed out in [4]. However, the composition of the two Newmark methods in (19) exhibits a much slower drift in the energy than DLA. At the moment, we have no explanation for this good behaviour. However, it is interesting to point out that the main advantage of using the composition method over the DLA method is obtained in the passenger energy. Although it exhibits a steadily increasing drift for the composition method (see Fig. 5(a)), it is much smaller than the observed drift for the DLA method. The cause of the random walk-type profile in the total energy is inherited from the driver energy (Fig. 5(b)), contrary to DLA and several other nonholonomic methods that nearly conserve it. This might be explained from the fact that the composition of nonholonomic Newmark methods is not preserving the Hamiltonian structure of the driver system. Although the Newmark method is very close from symplectic methods in the absence of constraints (see, e.g., [8]), the composition of Newmark methods seems to break down this close relationship. Interestingly, the passenger energy (Fig. 5(a)) exhibits a much slower drift than most nonholonomic methods (see [4]).

## 6. Future work

In a future paper, we will study the extension of the nonholonomic Newmark method to non-linear spaces, that is, in general differentiable manifolds. In particular, if  $Q = G$  is a Lie group we can derive a nonholonomic Lie–Newmark method (see [7]) where we assume that we have a retraction map  $R : \mathfrak{g} \rightarrow G$  (for instance the Lie group exponential map) and we identify by left (right)-trivialization  $TG \equiv G \times \mathfrak{g}$  with left (respectively, right)-trivialized coordinates  $(g, \xi)$ .



(a) Passenger energy for the pendulum-driven CVT,  $\epsilon = 0.1$ , as simulated using the composition Newmark method and the nonholonomic Leap-Frog method.



(b) Driver energy for the pendulum-driven CVT,  $\epsilon = 0.1$ , as simulated using the composition Newmark method and the nonholonomic Leap-Frog method.

**Fig. 5.** Simulation of driver and passenger energies.

Therefore if  $g_k \in G$  and  $\xi_k \in g_k^{-1}D_{g_k} \subseteq \mathfrak{g}$  then

$$g_k^{-1}g_{k+1} = R(h\xi_k + \frac{h^2}{2}\Gamma_{nh}(g_k, \xi_k, \lambda_k))$$

$$\frac{\xi_{k+1} - \xi_k}{h} = \frac{1}{2}\Gamma_{nh}(g_k, \xi_k, \lambda_k) + \frac{1}{2}\Gamma_{nh}(g_{k+1}, \xi_{k+1}, \lambda'_{k+1})$$

$$g_{k+1} \in \mathcal{M}_{g_k, h}^d, \quad \xi_{k+1} \in g_{k+1}^{-1}D_{g_{k+1}}$$

where we have also identified  $TTG \equiv G \times \mathfrak{g} \times \mathfrak{g} \times \mathfrak{g}$  and then  $\Gamma_{nh}(g_k, \xi_k, \lambda_k) \in \mathfrak{g}$  and  $\mathcal{M}_{g_k, h}^d$  is a discretization of the exact discrete constraint space.

**Data availability**

No data was used for the research described in the article.

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